Shock Waves in Quasicrystals

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Abstract

Shock waves in quasicrystals of the AlCuLi type and in approximant crystals of the C15 Laves phase have been studied by MD simulations. Three regimes are found: at low shock wave intensity the system reacts elastically, at high intensities it is turned amorphous. In the intermediate region we find a continuous transition with growing defective domains. The intensities where the behavior changes are different for the quasicrystal and the crystal, but the behavior itself is similar.

1. Introduction

Shock waves are a nice tool to expose a solid to strong uniaxial stress and to introduce defects without explicitly constructing them. Up to now, shock waves have been studied only in monatomic crystals to some depth[1]. There the shock stress is relaxed to a energetically more favorable hydrodynamically compressed state. Often stacking faults are created which permit a simple analysis of the results. For a crystal it is rather easy to construct slip planes and stacking faults and to analyze them. This is not the case for quasicrystals. If geometric constructions are used, complicated and rather arbitrary procedures have to be carried out to produce for example dislocations associated with extended defects.

Our first goal is to find out whether quasicrystals behave different than crystals if they are penetrated by shock waves. Many metals and alloys as well as fcc model crystals along the fourfold direction show a rather universal behavior with respect to the shock front velocity for example. We observe that this behavior is also valid for quasicrystals and binary crystals in the case of strong shock waves. For weak shock waves a deviation from the universal behavior is observed due to elastic precursor effects, and differences between the crystal and the quasicrystal are showing up. A similar behavior has been found recently for fcc crystals[2] in the two- and threefold directions.

Our second goal is to find out if new kinds of defects occur in the quasicrystal. By definition, a real shock wave in a crystal (as opposed to an elastic wave) causes permanent plastic deformation. Usually one finds stacking faults caused by slipping or twinning and martensitic deformations. In a quasicrystal these defects can occur also, but additional types of defects are possible: phason flips, phason walls, or transformations to crystals and approximants. It turns out that the types of defects in the quasicrystal are indeed different from those of the monatomic crystal, but similar to those in the binary crystal.

Up to now we have investigated only the transition from the elastic behavior to the plastic at medium shock wave intensities in detail. The low intensity range of the plastic behavior could not be studied until now due to the very long relaxation times involved in the transition from the elastic precursor state to the plastic final state.

2. Generation of the Shock Waves and Simulation Setup.

Shock waves have been generated in three-dimensional quasicrystals of the closed-packed Frank-Kasper-type which is realized in the Al-Cu-Li icosahedral quasi-crystals. The structure can be regarded as a quasiperiodic arrangement of oblate and prolate rhombohedra decorated with small A atoms at the corners and edge centers[3]. The large B atoms divide the diagonal of the prolate rhombohedron in the fraction $\tau{:}1{:}\tau$, with τ the golden mean $(1 + \sqrt{5})/2$. For comparison, simulations in a related cubic crystalline model, the C15 Laves phase of $MgCu_2$, have been carried out. The crystal phase can be regarded as a low-order approximant of the quasicrystal build of the prolate rhombohedra only. Both structures have a rather similar composition: The crystal has the structure formula A_2B, the composition of the quasicrystal is $A_{0.764}B_{0.236}$. The interactions were modeled by Lennard-Jones potentials. The radii of the potential minima have been adjusted to the shortest AA, AB and BB distances. The depth of the potentials between atoms of the same type is $-\epsilon$ and is -2ϵ between atoms of different types. The binding energy is 11.478ϵ for the quasicrystal and 12.974ϵ for the crystal.

There are a number of well established methods to generate shock waves in simulations[1]. In our case we have cut the sample into two halves and moved the parts against each other at constant velocities $\pm u_p$. Two shock waves are created at the center of the sample and move to the outside at velocities $\pm(u_s - u_p)$.

The standard molecular dynamics method was used for the simulations. The samples contained about 1,000,000 atoms. The geometry was a long rod of size $61{\times}61{\times}260$ in units of the minimal atomic distance a. The boundaries were open along the shock wave propagation direction and periodic along the two transverse directions. After the samples have been generated they were equilibrated for a time interval of $t = 10a\sqrt{m/\epsilon}$ (m the mass of the atoms) at $kT = 0.001\epsilon$ and pressure $P = 0.01\epsilon/a^1$.

3. Results

Quasicrystals should behave elastically isotropic whereas the Laves crystal should be anisotropic. To confirm this we have derived the elastic constants for a number of directions by quasistatic uniaxial deformation of the samples. The (quasi)-longitudinal velocity of sound is then given by $c_l = \sqrt{C/\rho}$ where C is the elastic constant and ρ is the density. For the Laves crystal we find a strong anisotropy: $c_{l4} = 14.07\sqrt{\epsilon/m}$, $c_{l3} = 12.61\sqrt{\epsilon/m}$, $c_{l2} = 13.00\sqrt{\epsilon/m}$. For the quasicrystal we get $c_{l2} = 12.41\sqrt{\epsilon/m}$, $c_{l3} = 12.48\sqrt{\epsilon/m}$, $c_{l5} = 12.40\sqrt{\epsilon/m}$. If all directions are taken into account we find an anisotropy for the Laves crystal of about 2% and of 0.2% for the quasicrystal. In the simplest case there should exist a linear relation between the velocity of the shock wave and the piston velocity $u_s = ku_p + b$,
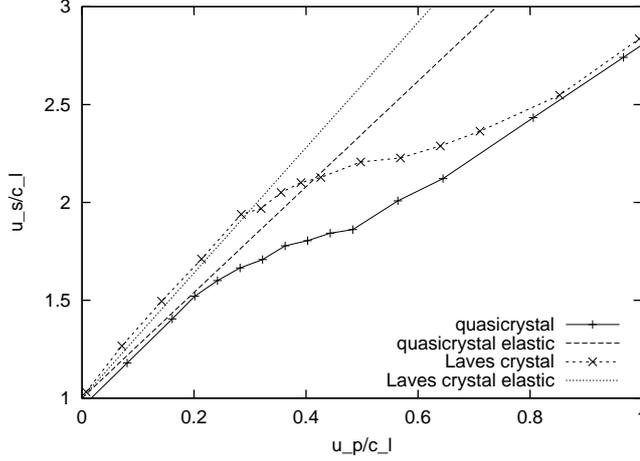
Figure 1: Shock vs. piston velocity. At low piston speed and at the beginning of the simulations we observe the elastic behavior, indicated by the straight lines. Between $u_p/c_l = 0.3$ and 0.6 we find a crossover to the plastic shock wave and the change of the slope to a materials-independent value.

where b should the longitudinal velocity of sound. The constants b derived in this way are very close to the velocities of sound obtained from the quasistatic computations for all directions that have been studied in the simulations.

Fig. 1 displays the u_s-u_p plot for Laves crystal and quasicrystal. At low piston velocities we observe unsteady elastic waves. This result is independent of the starting temperature of the sample. Between about 0.3 and about 0.6 u_p/c_l we find the crossover to plastic shock waves. At higher piston velocities we get a materials-independent plastic behavior and steady shock waves. The u_s vs. u_p curve obtained in our simulations does not depend on the sample cross-section and on the length of the rod as long as the shock wave has not penetrated the whole sample during simulation time. In the crystal the crossover from elastic to plastic behavior occurs at shock wave intensities higher than in the quasicrystal. The reason is that the local environment of an atom is on average more symmetrical in the crystal than in the quasicrystal.

The crystal structure remains largely perfect up to $u_p/c_l \approx 0.37$. Within a short interval of about $u_p/c_l = 0.1$ the behavior changes strongly. Defect bands occur which separate perfect domains. The bands grow with increasing strength of the shock wave. Starting at $u_p/c_l \approx 0.57$ the structure is destroyed completely by the shock wave. The quasicrystal stays intact up to a piston velocity of about $u_p/c_l = 0.25$. Only diffusion processes occur in this regime. Between $u_p/c_l = 0.25$ and 0.5 defect bands are observed as can be seen in Fig. 2. At shock waves stronger than $u_p/c_l = 0.5$ the quasicrystal becomes amorphous.

The width of the defects bands is up to $10a$ and the separation of the order of $35a$. The spacing between the bands depends on the cross section of the sample
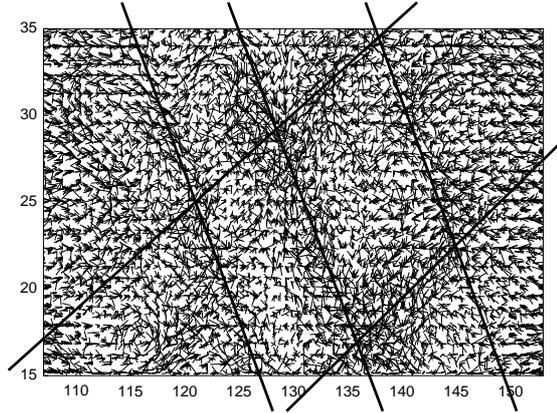
Figure 2: Pattern of defects in the quasicrystal at $u_p/c_l = 0.45$. A picture of the crystal would look quite similar.

since the bands are replicated by the periodic boundary conditions. In the case of small cross sections the boundary conditions may even mimic an amorphous state. A closer look at the bands shows that the samples break down into domains and layers which are rotated and shifted against one another. The defect bands are a transient phenomenon. If the samples are annealed after shocking they disappear, and the displacements become homogeneous.

4. Discussion

We have demonstrated that there is no deviation from the materials-independent relation between u_s and u_p in a C15 crystal and a diatomic quasicrystal in the case of strong shock waves. This is due to the complete destruction of the structures, a phenomenon which is well known from high-pressure studies of C15 phases. The reason is that it is not possible to exchange A and B atoms at random without destabilizing the structure and defects permitted in monatomic structures turn out to be fatal. In the case of weak shock waves, we find that the slopes for the quasicrystal and the crystal differ. The reason is the elastic behavior of the system where the structure plays a role. In the intermediate range we observe defect bands which mediate the stress relaxation. Contrary to the shear bands in fcc crystals[1] they are not sharp but several atomic distances thick.

The propagation direction of the shock waves was the four-fold direction in the crystal, and the two-fold direction in the quasicrystal normal to the close-packed planes. Simulations in other directions have also been carried out but cannot be presented here due to the limited space.

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